

SCOPE OF THE WORK

Reliance on CPU for communication limits scaling on GPU clusters

NVSHMEM provides GPU kernel-side OpenSHMEM API

NVLink is a high-bandwidth memory-like fabric between GPUs

Effectiveness of NVSHMEM over NVLink with Breadth First Search

CPU-initiated MPI vs GPU-initiated SHMEM in a particular implementation of BFS

AGENDA

GPU Programming Models: MPI and SHMEM

NVSHMEM Overview

DGX and NVLink

MPI+CUDA implementation of BFS

SHMEM implementation of BFS

Performance Evaluation

Conclusion and Future Work

GPU CLUSTER PROGRAMMING

Offload model

Compute on GPU
Communication from CPU

Synchronization at boundaries

Overheads on GPU Clusters
Offload latencies
Synchronization overheads

Limits strong scaling

More CPU means more power

```
void 2dstencil (u, v, ...)
 for (timestep = 0; ...) {
    interior_compute_kernel <<<...>>> (...)
    pack_kernel <<<...>>> (...)
    cudaStreamSynchronize(...)
    MPI_Irecv(...)
    MPI Isend(...)
    MPI_Waitall(...)
   unpack_kernel <<<...>>> (...)
   boundary_compute_kernel <<<...>>> (...)
```

GPU-CENTRIC COMMUNICATION

GPU capabilities

Warp scheduling to hide latencies to global memory Implicit coalescing of loads/stores to achieve efficiency

CUDA helps to program to these

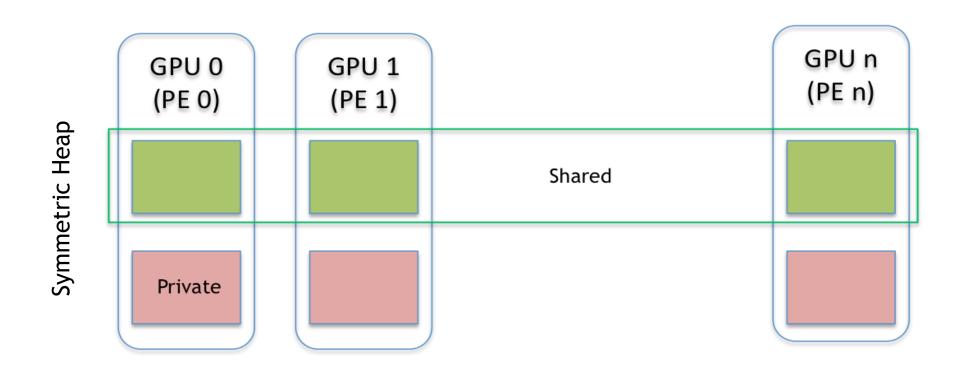
Should also benefit when accessing data over the network

Direct accesses to remote memory simplifies programming

Achieving efficiency while making it easier to program

Continuous fine-grained accesses smooths traffic over the network

GPU GLOBAL ADDRESS SPACE



COMMUNICATION FROM CUDA KERNELS

Long running CUDA kernels

Communication within parallelism

```
void 2dstencil (u, v, ...)
{
    stencil_kernel <<<...>>> (...)
}
```

```
__global__ void 2dstencil (u, v, sync, ...)
   for(timestep = 0; ...) {
      if (i+1 > nx) 
          v[i+1] = shmem_float_g(v[1], rightpe);
      if (i-1 < 1) {
          v[i-1] = shmem_float_g(v[nx], leftpe);
      u[i] = (u[i] + (v[i+1] + v[i-1]...
      if (i < 2) {
         shmem_int_p (sync + i, 1, peers[i]);
         shmem_quiet();
         shmem_wait_until (sync + i, EQ, 1);
     //intra-kernel sync
```

NVSHMEM

Implementation of OpenSHMEM Specification (1.3)

Symmetric heap on GPU memory

Implements multi-threading support as being discussed in PR #43

HOST ONLY

Library setup, exit and query Memory management

HOST/GPU

shmem_ptr

Remote memory access

Atomic memory operations

Collectives

Point-to-point synchronization

Memory ordering

Locking routines

Extensions for GPUs

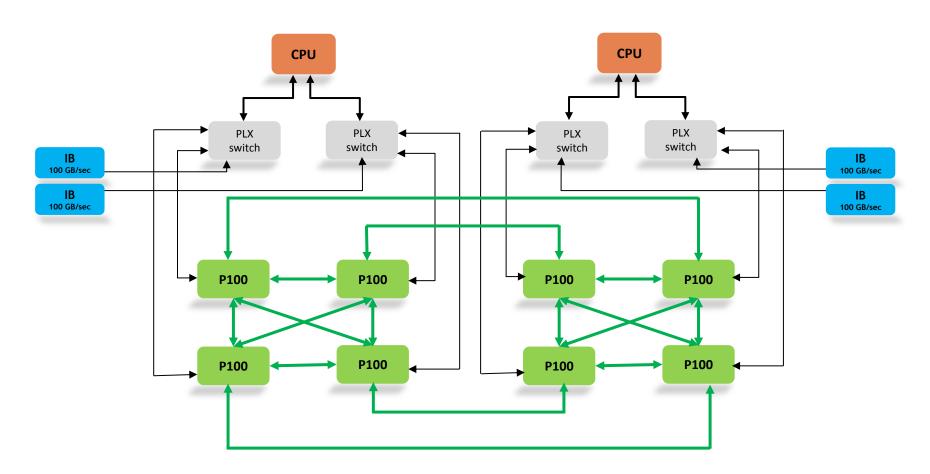
CUDA stream-based SHMEM communication

Thread cooperative SHMEM communication

Expected availability: Q4 2017 (single OS Multi-GPU nodes: NVLink, PCIe, QPI)



DGX-1 ARCHITECTURE

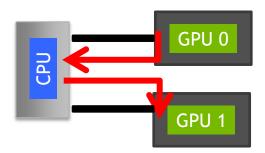


Inter-GPU Copies - Single Process

Unified Virtual Addressing available since CUDA 4.0 (2011)

```
cudaSetDevice(0);
cudaMalloc(&buf0, size)

cudaSetDevice(1);
cudaMalloc(&buf1, size)
------
cudaMemcpy (buf0, buf1, size, cudaMemcpyDefault )
```



GPUDirect P2P: by-passing CPU memory

cudaDeviceCanAccessPeer(int *access, int device, int peerdevice); cudaEnablePeerAccess(int peerDevice, unsigned int flags)

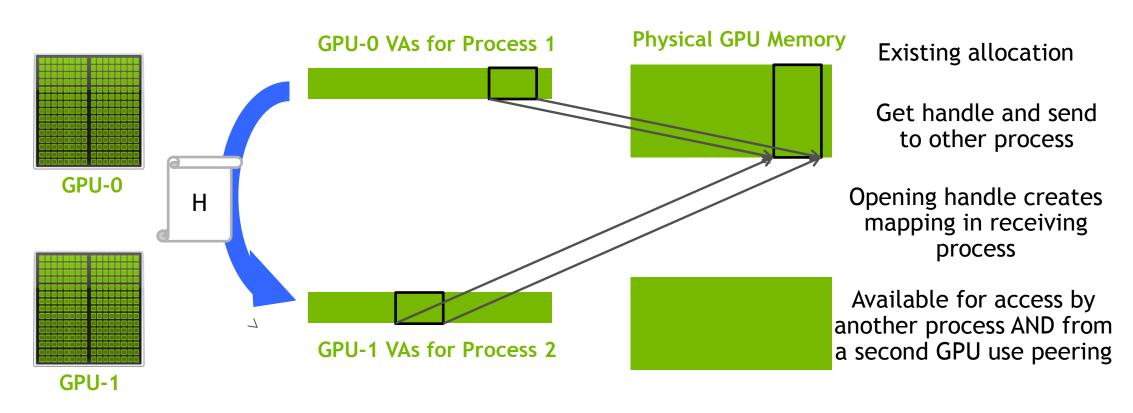
```
cudaSetDevice(0);
                                                                                            GPU 0
cudaMalloc(&buf0, size);
                                                                          CPU
                                                                                                           PCIe P2P
cudaCanAccessPeer (&access, 0, 1);
                                                                                                        (copy/LD/ST)
assert(access == 1);
                                                                                            GPU
cudaEnablePeerAccess (1, 0);
cudaSetDevice(1);
cudaMalloc(&buf1, size);
                                                                                             GPU
                                                                                                             NVLink
                                                                                                         (copy/LD/ST
                                                                                                           /atomics)
cudaSetDevice (0);
                                                                                            GPU
cudaMemcpy (buf0, buf1, size, cudaMemcpyDefault);
```

Can also access (LD/ST) the peer GPU memory from inside a CUDA kernel



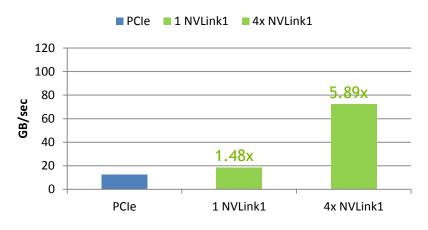
cudalpcGetMemHandle(), cudalpcOpenMemHandle() & cudaDeviceEnablePeerAccess()

Using GPU memory from another process

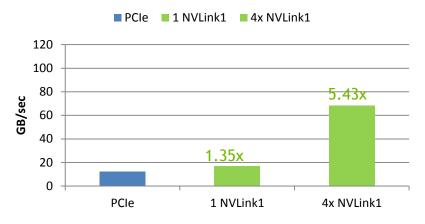


NVLINK1 W/ PASCAL

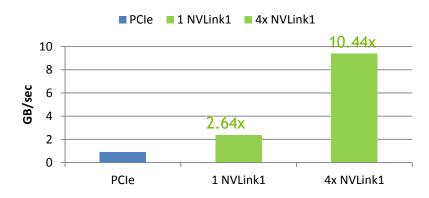
Copy using DMA



LD/ST - Linear



LD/ST - Random Access



- GPU memory model is relaxed and scoped
- Same memory model works within/across GPUs

BREADTH FIRST SEARCH (BFS)

Baseline: an MPI-based multi-GPU implementation of BFS by M.Bisson et. al.

Has been shown to scale to thousands of GPUs on the Tsubame supercomputer

Loosely follows the Graph 500 specification

R-MAT generator, mean performance over 64 BFS operations

Uses 32-bit vertices instead of required 48-bit representation

Uses a parallel level-synchronous algorithm

Frontier: list of vertices from which traversal starts in a give level

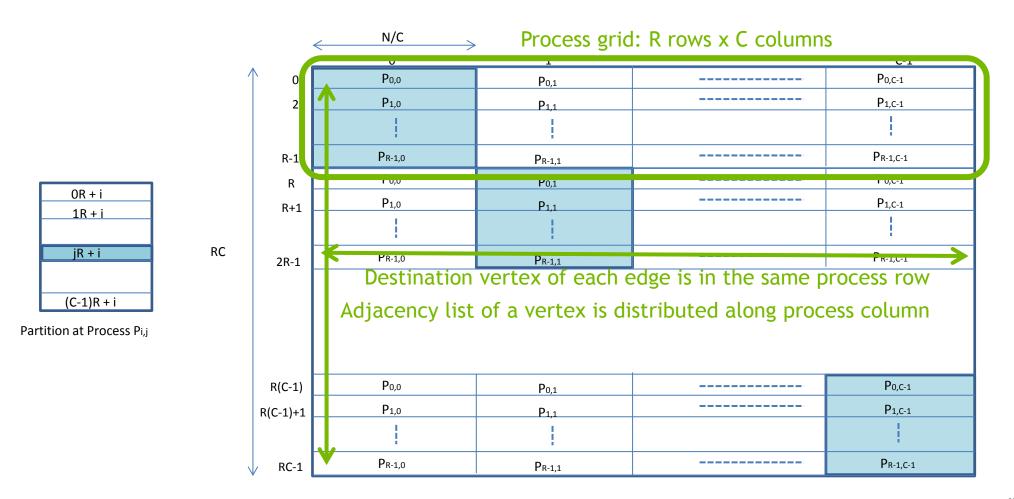
Expand: traverse graph to find un-visited neighbors of frontier vertices

Exchange: exchange list of newly found vertices

Append: remove redundancy and build the frontier for next level



DATA PARTITIONING



BFS USING MPI

frontier list at one processor column is populated with the seed vertex

```
while (frontier not empty)
{
    Expand: local expansion
    Horizontal Exchange: Alltoall exchange newly discovered vertices (happens only along grid rows)
    Append: build new frontier vertex list
    Vertical exchange: Allgather frontier list along grid columns (happens only along columns)
    Convergence check: Allreduce frontier list size among all processors
}
```

EXCHANGE USING MPI

Vertex lists are exchanged in two forms:

Using a vertex list (one integer per vertex)

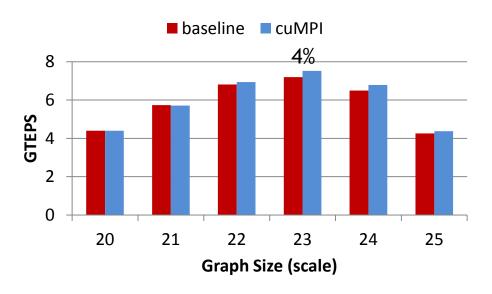
Using a bitmap (one bit per vertex)

Format is statically picked based on the level of traversal bitmap when number of discovered vertices is expected to be large vertex list when number of discovered vertices is expected to be large

Communication implemented using non-blocking MPI sends and receives

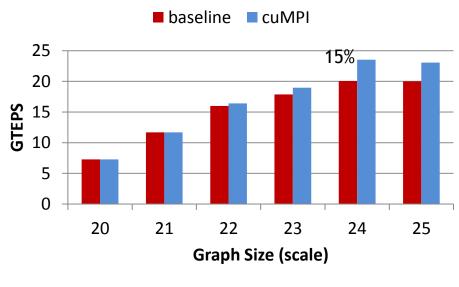
Enhanced the base version to using CUDA-aware MPI internally uses CUDA IPC/P2P to take advantage of direct PCIe or NVLink connections

PERFORMANCE WITH CUDA-AWARE MPI



4 K40 GPUs + PCle

Supermicro server w/ IvyBridge CPU and Broadcom PCIe switch, CUDA 8.0, MVAPICH2 2.2



4 P100 GPUs + NVLink

DGX-1 w/ Broadwell CPU, CUDA 8.0, MVAPICH2 2.2

BFS USING NVSHMEM

```
Fuse communication into CUDA kernels
     expand <- exchange of newly discovered vertices
      append <- exchange frontier vertices
while (frontier not empty)
  Expand on GPU: local expansion
  Append on GPU: build new frontier vertex list
  Convergence check on CPU: Allreduce frontier list size among all processors
     atomicOr(sbuf + r[k]/BITS(msk), m[k]);
      int peer = r[k] / drow_bl;
      uint32_t off = disp + r[k]%drow_bl;
      q[k] = shmem_int_or ((int *)(msk + off/BITS(msk)), m[k], peer);
```

gets rid of the MPI exchange code on the host

WORKAROUND FOR PCIE

GPU-GPU atomics are not supported over PCIE

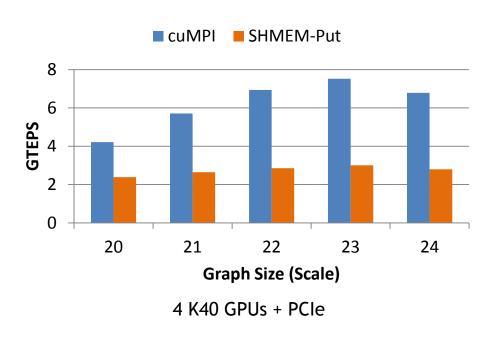
We take advantage of fact that 32-bit writes are atomic

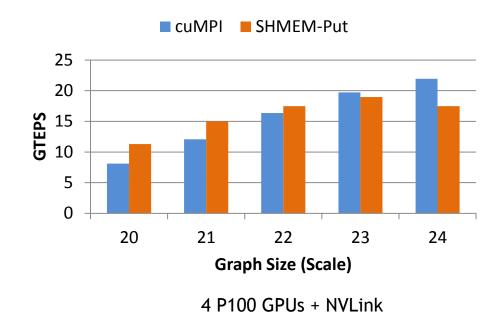
Vertex list is represented as integers, marked with shmem_int_p

Higher processing overhead as the vertex map is 32x larger

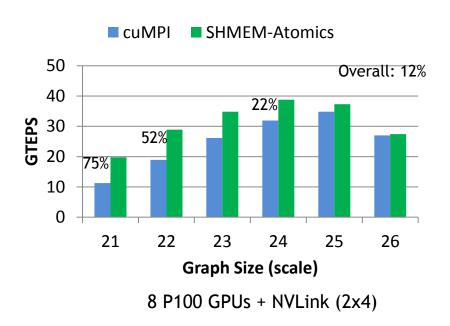
Provides a common version to compare behavior over PCIe and NVLink

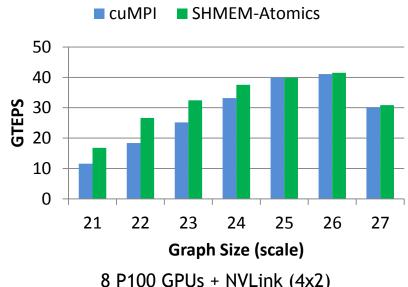
PERFORMANCE WITH PUTS





PERFORMANCE WITH ATOMICS





FUTURE WORK

Fairer comparison by removing tracking of predecessor information

Hybrid vertex list/bitmap design like in the case of MPI

Can offload multiple levels of BFS using stream-based collectives in NVSHMEM

Possibility of kernel fusion, using kernel-side collectives in NVSHMEM

Evaluate the use of IB to extend NVSHEM across multiple nodes

CONCLUSION

NVLink provides a high-bandwidth memory-like fabric between GPUS

NVSHMEM provides GPU-side communication API based on OpenSHMEM

We presented a study of using GPU-initiated communication in BFS

Benefits from reduced overheads in strong scaling cases, compared to using MPI

Tradeoff with efficient network utilization for weak scaling

THANKS

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Mauro Bisson, Massimo Bernaschi, Enrico Mastrostefano: Parallel Distributed Breadth First Search on the Kepler Architecture

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